m-Anisaldehyde, 6-hydroxy-672-13-9 | DTXSID40217478

Model Performance

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Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 7.47

Global applicability domain: Inside

Local applicability domain index: 6.75e-01

Confidence level: 4.20e-01

Nearest Neighbors from the Training Set

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Methylparaben Measured: 8.57 Predicted: 7.06 Image not found

1-Octanol Measured: 6.03 Predicted: 5.95 Image not found

Cyclohexanol Measured: 5.18 Predicted: 4.72

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1-Hexanol Measured: 5.18 Predicted: 4.67 Image not found

Phenacetin Measured: 9.59 Predicted: 9.23